PART 5

LM FOOD CHAIN

Chapter 3. Model Description

A food web bioaccumulation model usually consists of a series of submodels characterizing chemical bioaccumulation in each of the aquatic organisms in the food web. The individual submodels are linked together through feeding interactions among the organisms. The food web model (LM Food Chain) constructed for the Lake Michigan Mass Balance Project (LMMBP) is based on Version 5.2 of the computer model FDCHAIN which was originally developed by HydroQual, Inc., Mahwah, New Jersey. The original model and its early versions have been previously applied in numerous projects including the Green Bay Mass Balance Food Chain Modeling project (Connolly *et al.*, 1992). Several additions and modifications have been made to enhance the performance of the food web model. They include the introduction of a multi-compartment approach to better accommodate the spatially variable conditions in Lake Michigan, refinements of certain parameters to reflect advancements of knowledge in related disciplines, the incorporation of a new submodel for chemical bioaccumulation of benthic invertebrates, and the integration of alternative modeling equations for species-specific parameters that are not readily obtainable. The following is a detailed description of submodels used in the LM Food Chain for simulating organic chemicals in individual fish and in organisms of lower trophic levels of fish food webs.

5.3.1 Chemical Bioaccumulation in Fish

The model is a set of equations derived using the principle of mass conservation. It is generally accepted that the primary processes of chemical exchange between a fish and its exposure environment are: 1) chemical uptake from water, 2) chemical uptake from food sources, 3) chemical elimination due to respiration and excretion, and 4) chemical concentration reduction by growth dilution (Figure 5.3.1). The submodel for chemical bioaccumulation in fish can then be derived based on a simple mass balance equation for chemicals in the fish. The general form of the mass balance equation is well-defined. The rate of change in chemical concentration in a fish (dC_F/dt) is equal to the sum of the relevant chemical fluxes into and out of the fish.

$$dC_F/dt = F_w + F_p - F_e - F_g \qquad (5.3.1)$$

where

dC_F/dt = chemical increment in fish per unit time (μg/kg/day)

F_w = flux of chemical uptake from water (μg/kg/day)

F_p = flux of chemical uptake from prey items (μg/kg/day)

F_e = flux of chemical elimination *via* respiration (μg/kg/day)

F_g = flux of chemical reduction by growth dilution (μg/kg/day)

In some cases, other chemical fluxes, such as flux associated with the chemical elimination through metabolism transformation in the organism, may also need to be included in Equation 5.3.1. In this study,

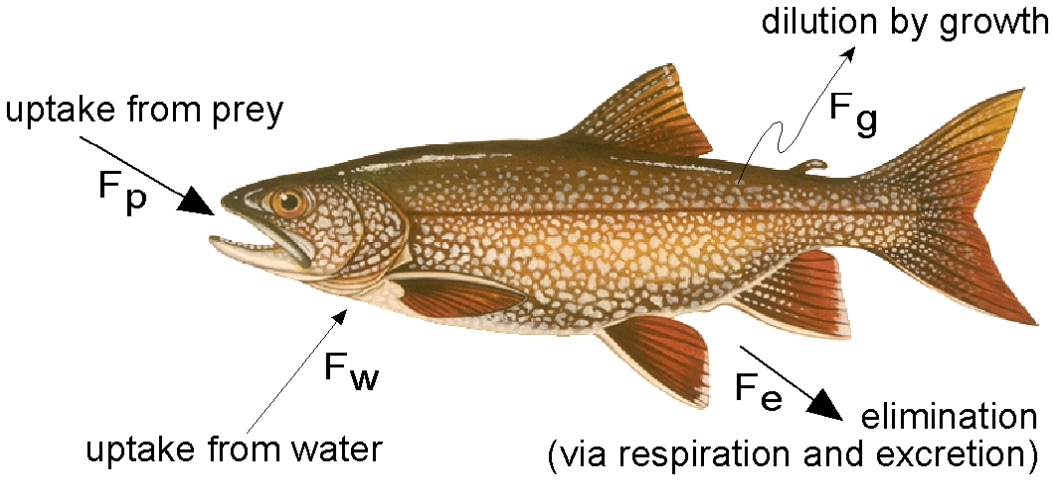

Figure 5.3.1. Primary chemical exchange processes between a fish and its environment.

we assumed that metabolism transformation of polychlorinated biphenyl (PCB) contaminants was negligible (Gobas, 1993; Stapleton *et al.*, 2001; U.S. Environmental Protection Agency, 1999).

After construction of the mathematical description for each of the chemical fluxes in the mass balance equation, the chemical concentration in the fish C_F (µg-chem/kg-body) at time t + Δt was then calculated by numerical integration:

$$C_F(t + \Delta t) = C_F(t) + [dC_F(t)/dt] \cdot \Delta t \qquad (5.3.2)$$

To predict chemical bioaccumulation for top predator fish, the mass balance equation was repeatedly applied to organisms at each trophic level to simulate chemical biomagnification from forage species to top predators.

Several methods have been developed to describe chemical dynamics in fish and to estimate related chemical fluxes in the mass balance equation. In this food web bioaccumulation model, the chemical dynamics were described based on fish bioenergetics (Lantry and Stewart, 1993; Rudstam, 1989; Rudstam *et al.*, 1994; Stewart *et al.*, 1983; Stewart and Binkowski, 1986). The mathematical equation used to estimate the chemical fluxes in the mass balance equation are described below.

5.3.1.1 Chemical Uptake From Water

The chemical flux entering an organism from water *via* gill ventilation (F_w) is expressed as a product of the fish's ventilation rate and the dissolved chemical concentration in water. The extent to which chemicals that enter the gill compartment by gill ventilation and are actually absorbed by the fish is usually expressed by the chemical gill transfer coefficient, E_c, which is included in F_w.

$$F_w = E_c \cdot K_v \cdot C_w \qquad (5.3.3)$$

where

E_c = chemical gill transfer coefficient

K_v = gill ventilation rate (L-water/kg-fish/day)

C_w = dissolved chemical concentration in water (µg-chem/L-water)

The gill ventilation rate of a fish (K_v) is dependent on the amount of oxygen required by the fish to sustain its normal respiration (R_o) and the oxygen content in the water that passes through the gill membrane.

$$K_v = R_o/(E_o \cdot [O_2]) \qquad (5.3.4)$$

where

R_o = rate of oxygen uptake from water, or fish respiration rate (mg-O_2/kg-fish/day)

E_o = oxygen gill transfer coefficient

$[O_2]$ = oxygen content in water (mg-O_2/L-water)

Similarly, the oxygen gill transfer coefficient, E_o reflects the extent to which oxygen that enters the gill compartment by gill ventilation is actually absorbed by the fish. The value of R_o, which is expressed in terms of oxygen consumption, can usually be calculated using a bioenergetics model (Hewett and Johnson, 1989). Oxygen content in water $[O_2]$ was estimated as a function of water temperature based on an empirical equation for oxygen saturation in water (Greenberg *et al.*, 1992).

Substituting Equation 5.3.4 into Equation 5.3.3, the chemical flux *via* gill uptake from water (F_w) then follows as

$$F_w = (E_c/E_o) \cdot (R_o/[O_2]) \cdot C_w \quad (5.3.5)$$

5.3.1.2 Chemical Uptake From Prey

The chemical flux absorbed by fish from diet (F_p) *via* the gastrointestinal tract is expressed using the food ingestion rate of the fish (K_f) and chemical concentration in its diet (C_p). The extent to which chemicals in the diet are actually absorbed by the fish can be expressed by the chemical assimilation efficiency α, which is included in F_p.

$$F_p = \alpha \cdot K_f \cdot C_p \quad (5.3.6)$$

where

α = chemical assimilation efficiency

K_f = food ingestion rate (g-prey/g-body/day)

C_p = chemical concentration in prey (µg-chem/g-food)

The chemical concentration in the diet (C_p) is based on diet composition and chemical content in each prey component. The food ingestion rate is determined by an energy balance. The energy intake from food sources is equal to the energy expenditure of the fish for respiration and growth:

$$(K_f \cdot D_p) \cdot \beta = R \cdot D_F + G \cdot D_F \quad (5.3.7)$$

where

D_p = energy density of prey (kJ/kg-prey)

D_F = energy density of the fish (kJ/kg-body)

R = fish respiration rate (kg-fish/kg-body/day)

G = fish growth rate (kg-fish/kg-body/day)

β = fraction of ingested energy that is assimilated

R can usually be calculated using a fish bioenergetics model (Hewett and Johnson, 1989). G can be estimated by individual fish weight-age relationships. The energy density (D_F and D_p) can be estimated from the lipid and protein content of the fish and prey. Substituting Equation 5.3.7 into Equation 5.3.6, the flux of chemical uptake *via* food consumption, F_p, can be formulated as follows:

$$F_p = (\alpha/\beta) \cdot (D_F/D_p) \cdot (R + G) \cdot C_p \quad (5.3.8)$$

5.3.1.3 Chemical Elimination *Via* Gills

The flux of chemicals eliminated by a fish *via* the gills is expressed as a product of gill elimination rate constant, K_e, and chemical concentrations in the organism, C_F:

$$F_e = K_e \cdot C_F \quad (5.3.9)$$

where

K_e = gill elimination rate constant (1/day)

C_F = chemical concentration in organism (µg-chem/kg-body)

Because the elimination is, in essence, the reverse process of gill uptake, the gill elimination rate constant can be related to the gill uptake rate constant. If we view the ratio of gill uptake and elimination rate constants as the chemical partition coefficient between the body tissue and aqueous

phases of the organism, the gill elimination rate constant can then be derived as

$$K_e = (E_c \cdot K_v) \cdot \rho/(f_a + f_L \cdot \pi) \quad (5.3.10)$$

where

E_c = chemical gill transfer coefficient

K_v = gill ventilation rate (L-water/kg-body/day)

ρ = aqueous phase density of the organism (kg/L)

f_a = non-lipid fraction of the fish

f_L = lipid fraction of the fish

π = chemical partition coefficient between lipid and non-lipid phases of the organism

Substitution of Equation 5.3.10 into Equation 5.3.9 yields an equation for estimating the flux of chemicals eliminated from the fish *via* gill ventilation:

$$F_e = C_F \cdot (E_c \cdot K_v) \cdot \rho/(f_a + f_L \cdot \pi) \quad (5.3.11)$$

For most organic chemicals, gill elimination is a major mechanism of chemical discharge from fish (Gobas *et al.*, 1989). Fecal elimination and excretion of chemicals are not specifically modeled in this mass balance equation. Their contribution can be viewed as having been factored into the food of chemical assimilation efficiency and gill transfer coefficient.

5.3.1.4 Chemical Dilution by Growth

Fish growth results is an increase of the fish volume and a reduction of chemical mass per fish volume. The equivalent flux of chemical loss due to fish growth (F_g) is expressed as a product of the fish growth rate (G) and chemical concentration in the fish (C_F).

$$F_g = G \cdot C_F \quad (5.3.12)$$

where

G = growth rate of organism (1/day)

C_F = chemical concentration in fish (µg-chem/kg-body)

The fish growth rate (G) was estimated based on fish weight-age relationships established for each fish species.

5.3.2 Chemical Bioaccumulation in the Base of Food Webs

The aquatic species at the base of the Lake Michigan food web are zooplankton (pelagic) and *Diporeia* (benthic). The modeled equations discussed above for individual fish can not be applied to zooplankton and *Diporeia* due to the lack of species-specific bioenergetics data. Alternative submodels are needed for chemical bioaccumulation in the base of the food webs.

5.3.2.1 Chemical Bioaccumulation in Zooplankton

Zooplankton in the Lake Michigan food webs are a mixture of a wide variety of species. The species composition of the zooplankton is not fixed. It varies with season depending on the optimal temperature for the growth of individual species. It is also dependent on prey selections of its predators in a given food web. At this stage, it is unfeasible to develop a kinetic submodel for this species group due to the lack of appropriate information.

For simplicity, a steady-state model was adapted in our food web models to calculate concentrations in Lake Michigan zooplankton. In this chemical bioaccumulation submodel, zooplankton were assumed to be a homogeneous pseudo-species. Under steady-state, the chemical mass balance Equation 5.3.1 can then be expressed as

$$F_w + F_p - F_e - F_g = 0 \quad (5.3.13)$$

The parameters in this equation have the same definition as those in the fish submodel. Substituting Equations 5.3.3, 5.3.6, 5.3.9, and 5.3.12 into Equation 5.3.13, the chemical concentration in zooplankton C_z can then be calculated by the following equation.

$$C_z = (K_c \cdot K_v \cdot C_w + \alpha \cdot K_f \cdot C_p)/(K_e + G) \quad (5.3.14)$$

5.3.2.2 Chemical Bioaccumulation in *Diporeia*

There are several experimental studies on chemical uptake from sediments by *Diporeia* (Landrum, 1989; Landrum *et al*., 1985). Because most of the studies were conducted under controlled laboratory conditions, the kinetics of chemical exchange between *Diporeia* and its environment derived from these studies can not be readily transformed into a kinetic model applicable to a real system. The lack of information on site-specific growth data and the difficulty in characterizing the surface sediment portion that is actively selected by *Diporeia* as a food source also hindered the development of a kinetic model for chemical bioaccumulation in *Diporeia*.

The submodel for chemical bioaccumulation in *Diporeia* used in this food web model was based on a published steady-state model for benthic animals. This model, introduced by Morrison *et al*. (1996), assumes that under a steady-state condition the total chemical intake flux from water (U_w) and food (U_d) by a benthic animal equals the total chemical elimination flux from the animal *via* gill (D_w), faeces (D_f), and metabolism (D_m):

$$U_w + U_d = D_w + D_f + D_m \qquad (5.3.15)$$

For detrivores, this assumption yields the equation:

$$(f_b/f_s) = [E_w \cdot G_w \cdot (f_w/f_s) + E_d \cdot G_d \cdot (f_d/f_s) \cdot DS_d \cdot OC_d \cdot K_{oc}] / /[E_w \cdot G_w + E_d \cdot (1 - \alpha) \cdot (1 - \beta) \cdot G_d \cdot DS_d \cdot OC_d \cdot K_{oc} + V_b \cdot k_m \cdot K_{bw}] \qquad (5.3.16)$$

where

f_b = chemical fugacity in benthos, Pa

f_s = chemical fugacity in sediment, Pa

f_d = chemical fugacity in diet (sediment or suspended particles), Pa

E_w = chemical assimilation efficiency from water

G_w = gill ventilation rate, L/day

E_d = chemical assimilation efficiency from diet

G_d = food ingestion rate, L (wet volume)/day

DS_d = density of diet (wet), kg/L

OC_d = organic carbon fraction of diet on wet weight base

K_{oc} = organic carbon-water partition coefficient, L/kg

α = organic carbon assimilation efficiency

β = fraction of ingested diet absorbed

V_b = volume of benthic animal, L

k_m = chemical metabolic transformation rate in benthic animal, 1/day

K_{bw} = benthos-water partition coefficient of chemicals, L/L

With mathematical manipulation and necessary unit conversion, the chemical fugacity terms (f_b/f_s), (f_w/f_s) and (f_d/f_s) in this model equation can be replaced by some more readily available chemical parameters. The submodel for chemical bioaccumulation in benthic animals can then be expressed as:

$$C_B = (E_w \cdot G_w \cdot C_w + E_d \cdot G_D \cdot C_D) \cdot L_b \cdot K_{ow} / /[E_w \cdot G_w \cdot 1000 + E_d \cdot (1 - \alpha)(1 - \beta) \cdot G_d \cdot K_{oc} + W_b \cdot k_m \cdot K_{ow}] \qquad (5.3.17)$$

where

C_B = chemical concentration in fresh benthic animal, µg/g-wet

C_D = chemical concentration in diet (organic carbon normalized), µg/g-OC

G_D = food ingestion rate, g-OC/day

W_b = body weight of fresh benthic animal, gram

L_b = lipid fraction in fresh benthic animal

5.3.3 Model Description of Exposure Environment

Calculations in the submodels discussed above require information which characterizes the environmental conditions for individual organisms, such as environmental temperature, oxygen content, and the contaminant levels in water (for pelagic species) and sediment (for benthic species). These data are essential for application of a food web bioaccumulation model.

However, among all existing aquatic food web models the environmental condition of a food web is typically defined with a single spatial compartment. This makes no distinction of preferred living condition among individual organisms and implies that all organisms in a food web live in an uniform environment. This simplified model approach is adequate for food webs in shallow and small water bodies where gradients are relatively small, and thus the exposure environments are expected to be similar among organisms in different trophic levels on a seasonal basis. However, for food webs in a large aquatic system, such as Lake Michigan, the single spatial compartment approach for defining exposure environment of a food web may not be adequate.

In Lake Michigan, the spatial variation in water temperature can be substantial, especially during summer stratification (Ayers, 1962; Brandt *et al.*, 1991; Carr, 1973; Sommers *et al.*, 1981). As a result, organisms in the lake are exposed to different temperatures depending on individual temperature preferences (Brandt *et al.*, 1980; Otto *et al.*, 1976). Species living in surface water are exposed to a temperature that varies dramatically from season to season. Species living in deep water are exposed to a relatively stable temperature. There are also species that prefer different environments at different life stages. The exposure temperatures of these species are expected to vary by age (Lantry and Stewart, 1993; Stewart and Binkowski, 1986). It is therefore, possible for a food web to consist of predators and prey that have different exposure temperatures. It appears that existing food web model frameworks are not adequately formulated to accommodate the differential exposure temperatures among organisms in Lake Michigan food webs.

To better represent the exposure environment for each component of a food web and thus, to reduce the associated uncertainties in model estimates, a multi-compartment approach was introduced in the food web model framework. Unlike the original single compartment modeling approach which models the exposure condition as a homogeneous one for the whole food web, the multi-compartment approach allows modelers to define the exposure conditions individually for each organism with separate spatial compartments. Each compartment can be assigned organism-specific parameters which reflect the environmental condition of the preferred location of the associated organism. The temporal variation of the preferred location of the organism can be represented by the corresponding change in the parameters of the compartment over time. Figure 5.3.2 provides the conceptual diagrams for both the original single compartment approach and the new multi-compartment modeling approach. For the modified model approach, the differential exposure temperatures among the organisms in a food web can be easily described by defining each organism with an independent spatial compartment.

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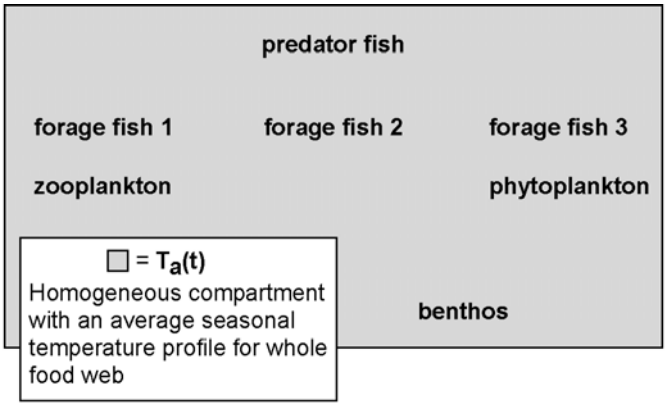
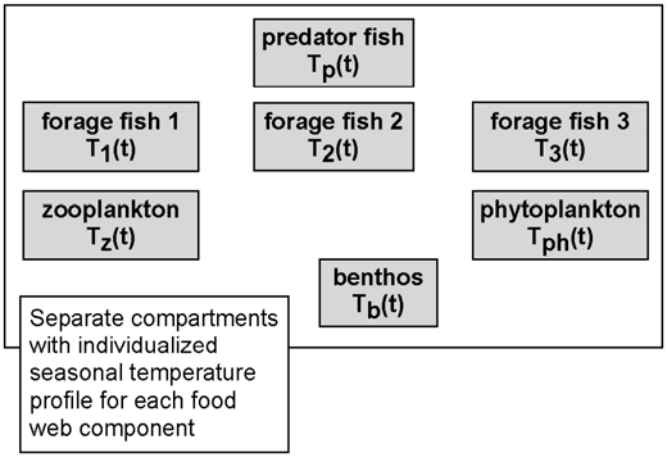


A. Single compartment approach for exposure temperature in existing food chain models.



B. Multi-compartment approach for exposure temperature in food chain models.

Figure 5.3.2. Comparison of modeling approaches for exposure temperatures in food web models.

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